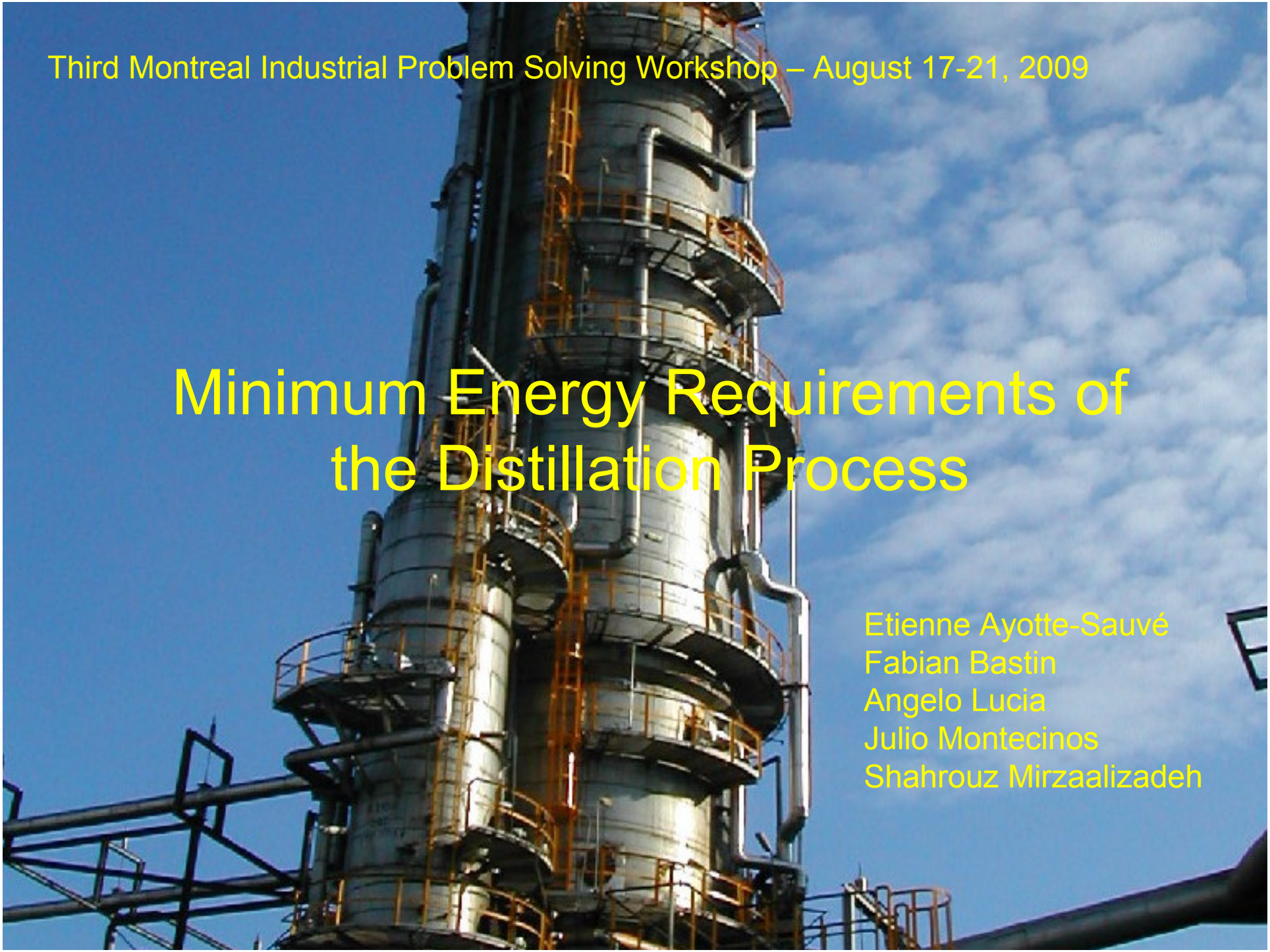

Third Montreal Industrial Problem Solving Workshop – August 17-21, 2009

Minimum Energy Requirements of the Distillation Process

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Outline

1. Foreword
2. Problem statement
3. Solution approach
4. Future work

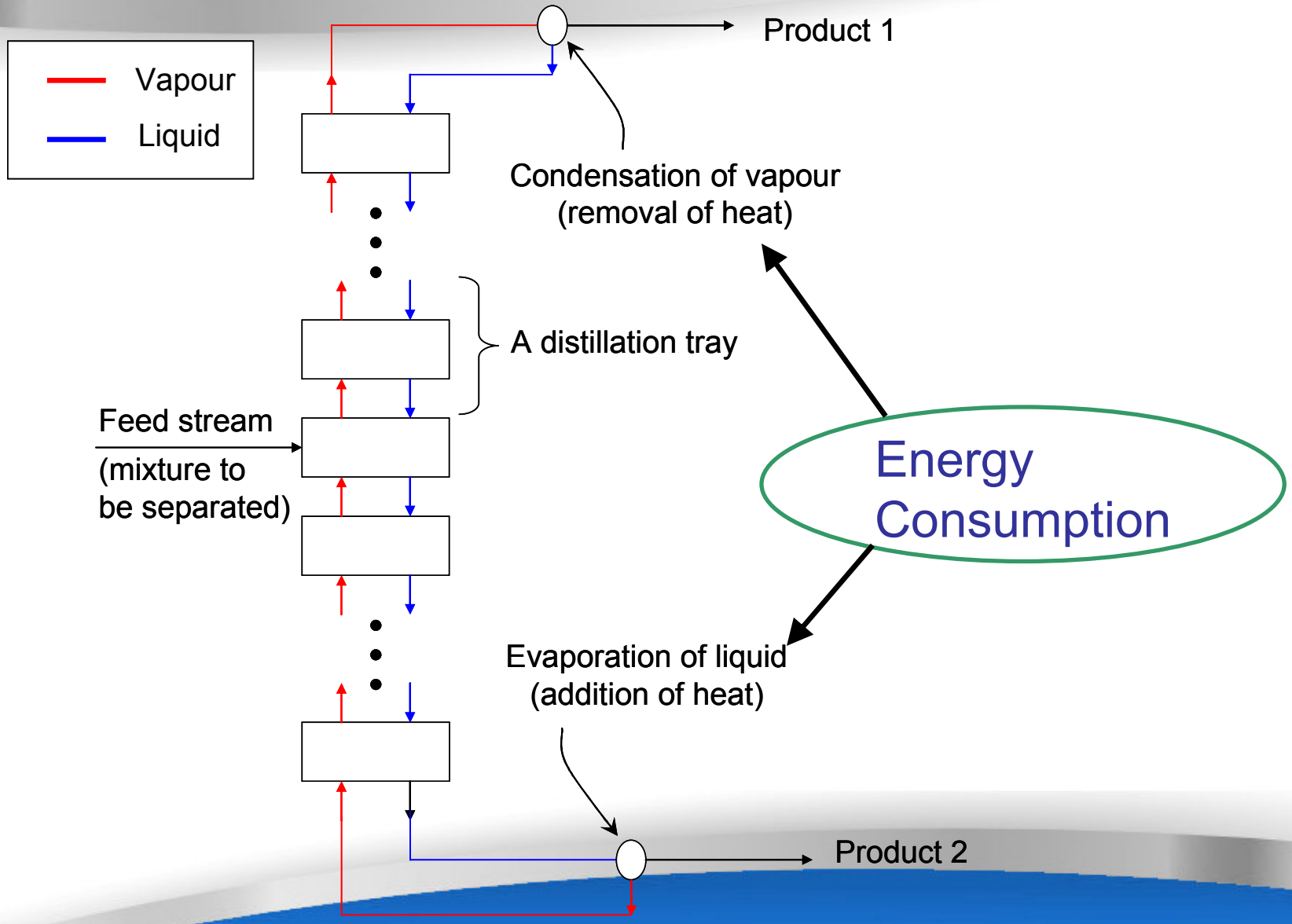
1. Foreword

- Of all know separation processes, distillation is arguably the most energy intensive and the most widespread.
- There are approximately 40 000 distillation columns in the US alone (source: DOE study, 2005).
- These columns account for 18% of the total energy consumption in the whole US manufacturing sector (source: DOE study, 2005).
- Similar numbers are expected for Canada.
- Separation needs continue to be addressed via distillation (best compromise to date between product purity and process throughput).

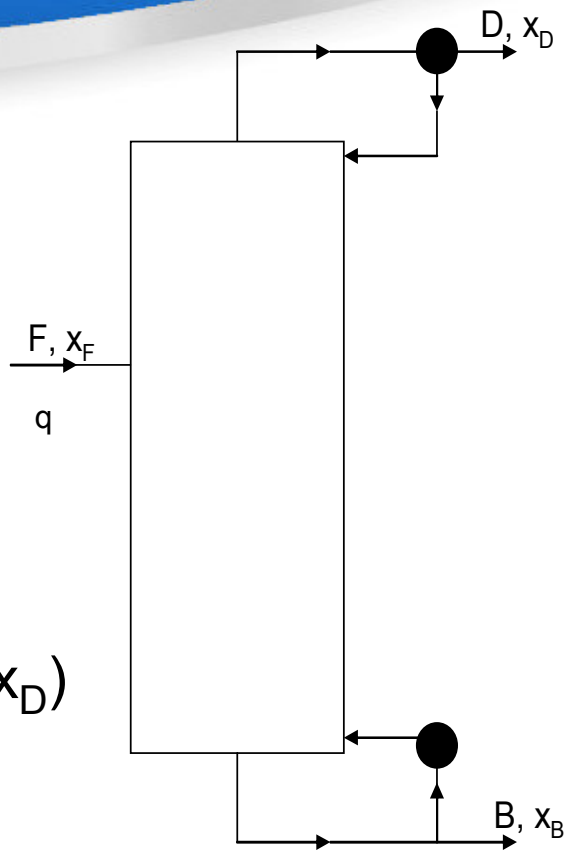
Thus, determining the minimum energy requirements of distillation is important.

2. Problem Statement

What is distillation ?



Problem Statement



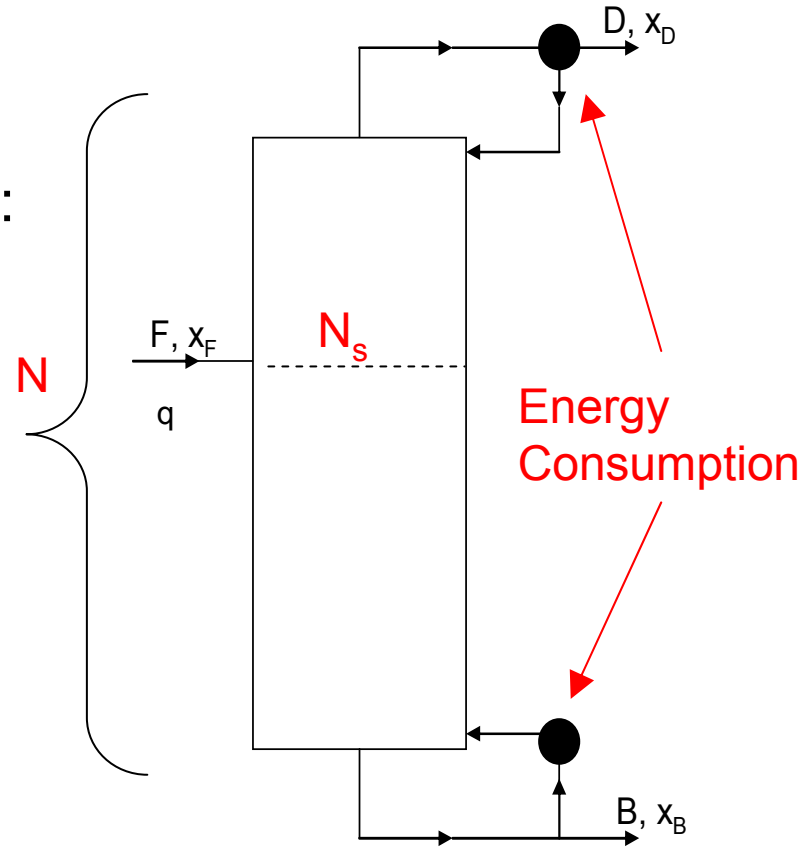
Given a *separation task*, i.e. given:

- the thermal state of the feed (q)
- the feed flow rate (F) and composition (x_F)
- the bottoms composition (x_B)
- a target value of the distillate composition (x_D)

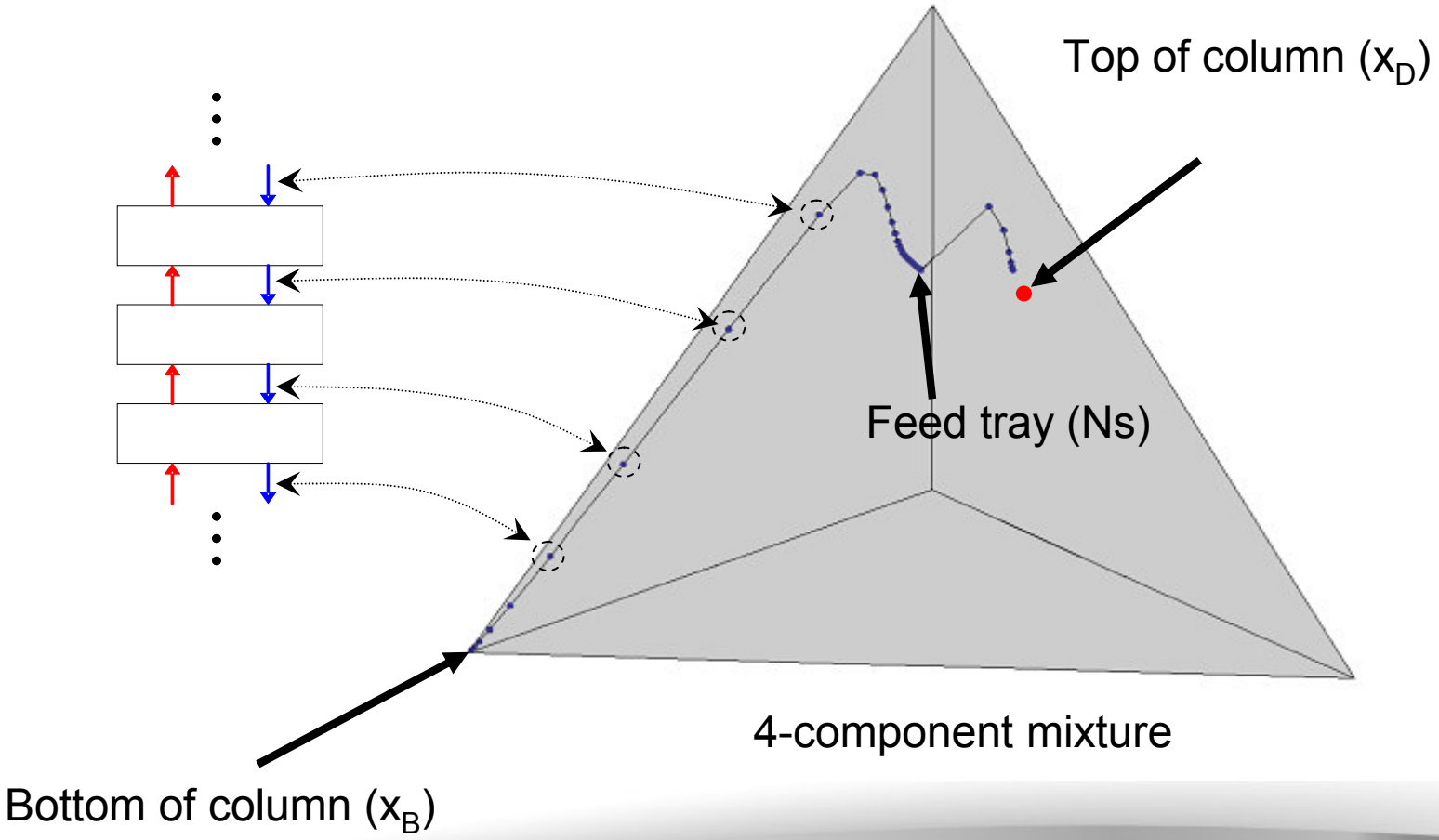
determine the minimal energy consumption for which this separation task can be achieved while obtaining a distillate composition in a neighbourhood of the specified x_D.

Degrees of freedom (decision variables):

- Energy consumption of the column
- Total number of trays (N)
- Position of the feed stream (Ns)



Sequence of liquid composition vectors for a given energy consumption.



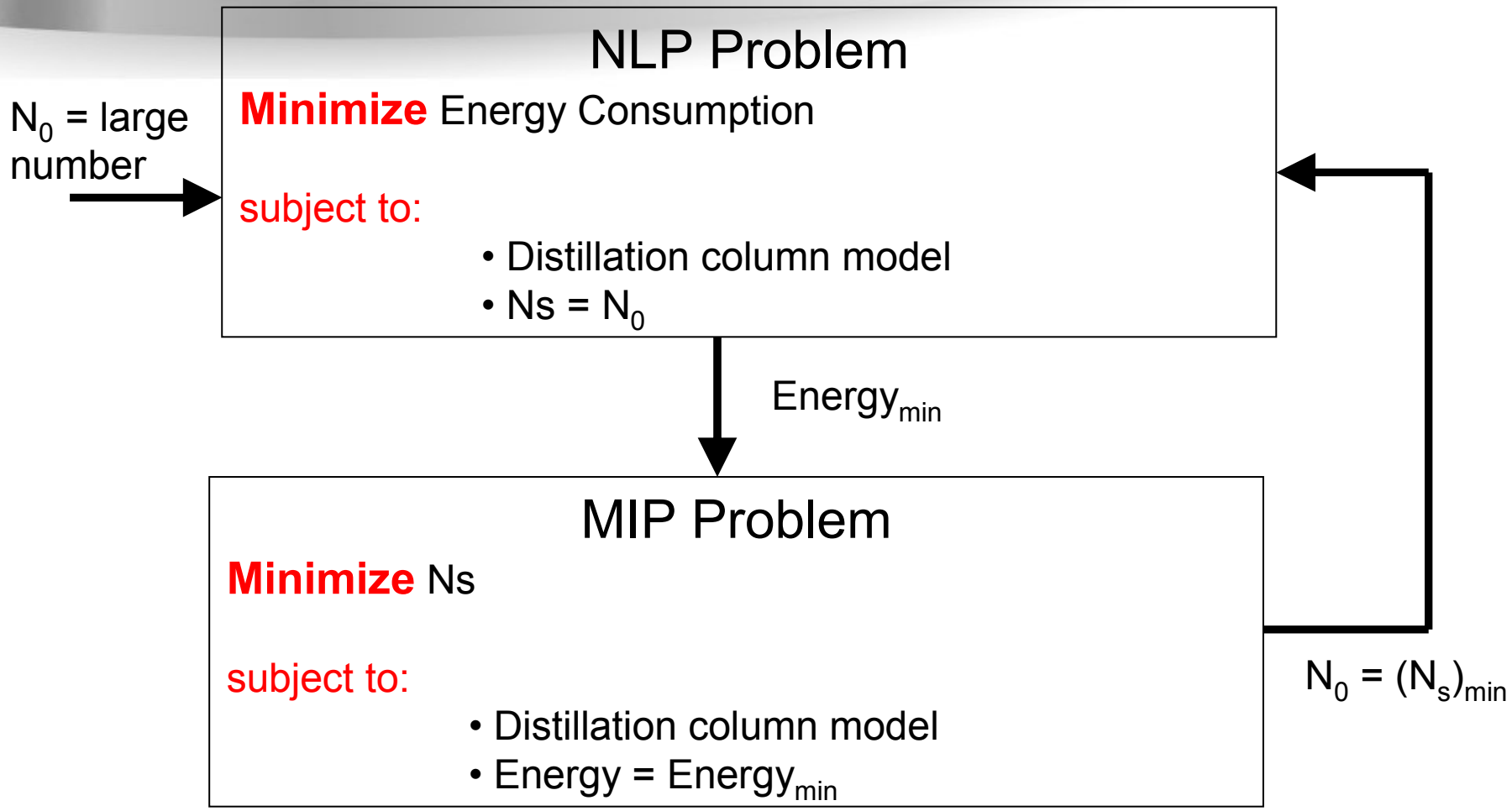
Challenges

• Excluding certain non-ideal mixtures (which have not proven to be industrially relevant to this day), minimum energy requirements are reached asymptotically when the number of distillation trays grows to infinity.

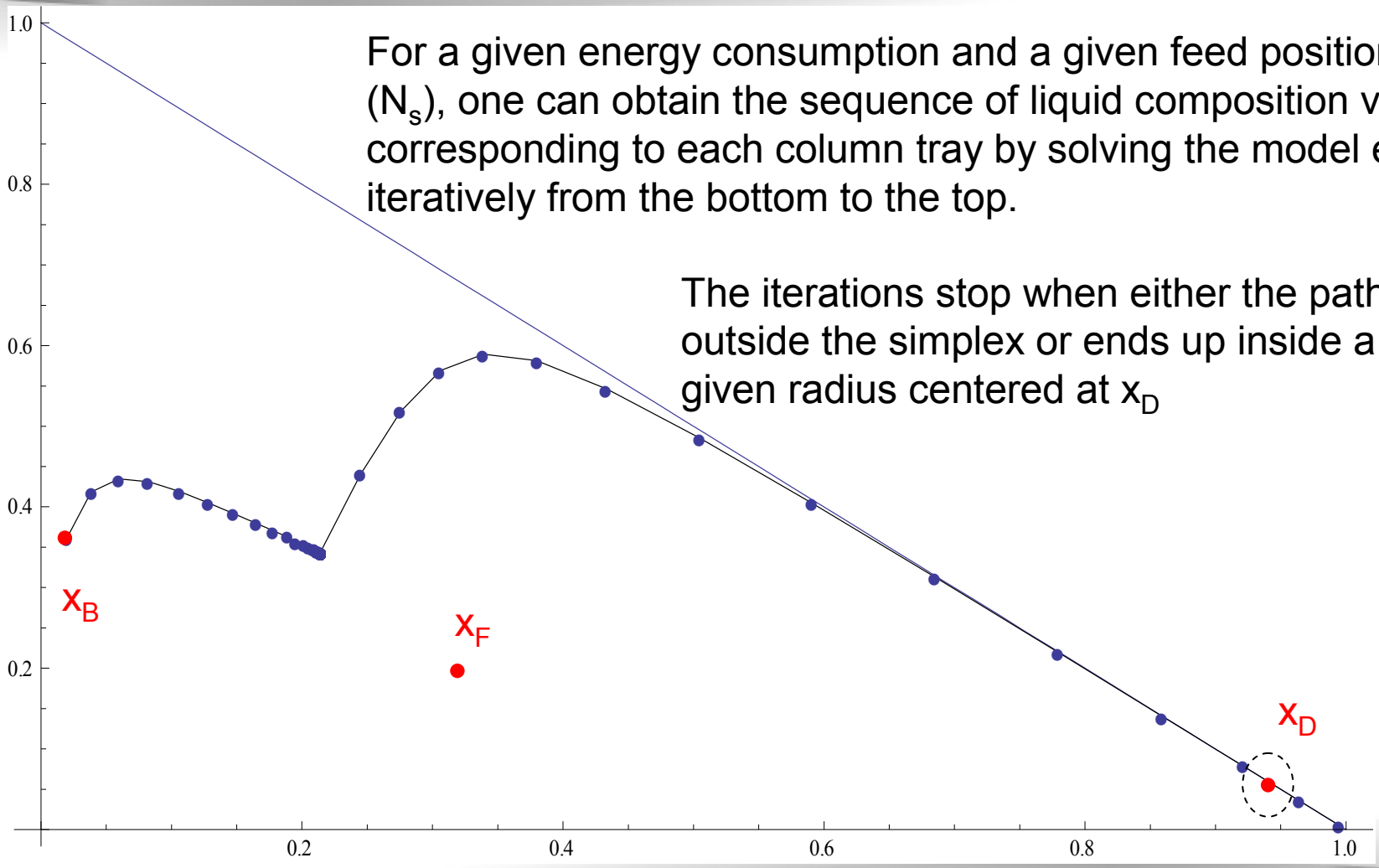
• One approach to address this issue, is to split the MINLP problem in two:

  • Try to find a minimal energy solution for an infinite number of trays ($N_s \longrightarrow$ infinity)

  • Try to see if the number of trays can be reduced for the given solution obtained in the previous step.


NLP Problem
Minimize Energy Consumption
subject to:
• Distillation column model
• Ns = N0
N0 = large number
Energymin
MIP Problem
Minimize Ns
subject to:
• Distillation column model
• Energy = Energymin
N0 = (Ns)min

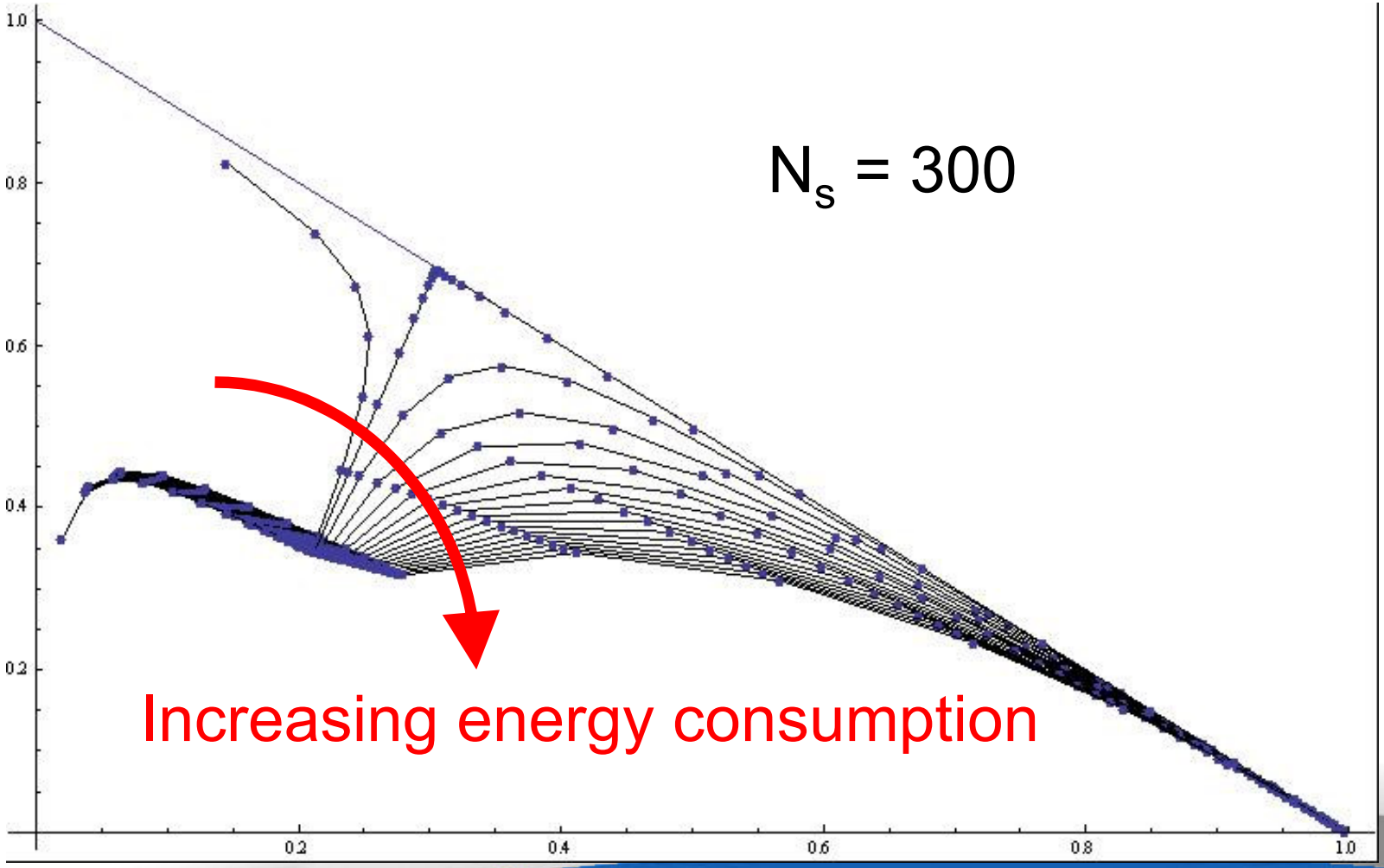
Remark



For a given energy consumption and a given feed position (N_s), one can obtain the sequence of liquid composition vectors corresponding to each column tray by solving the model equation iteratively from the bottom to the top.

The iterations stop when either the path goes outside the simplex or ends up inside a ball of given radius centered at x_D

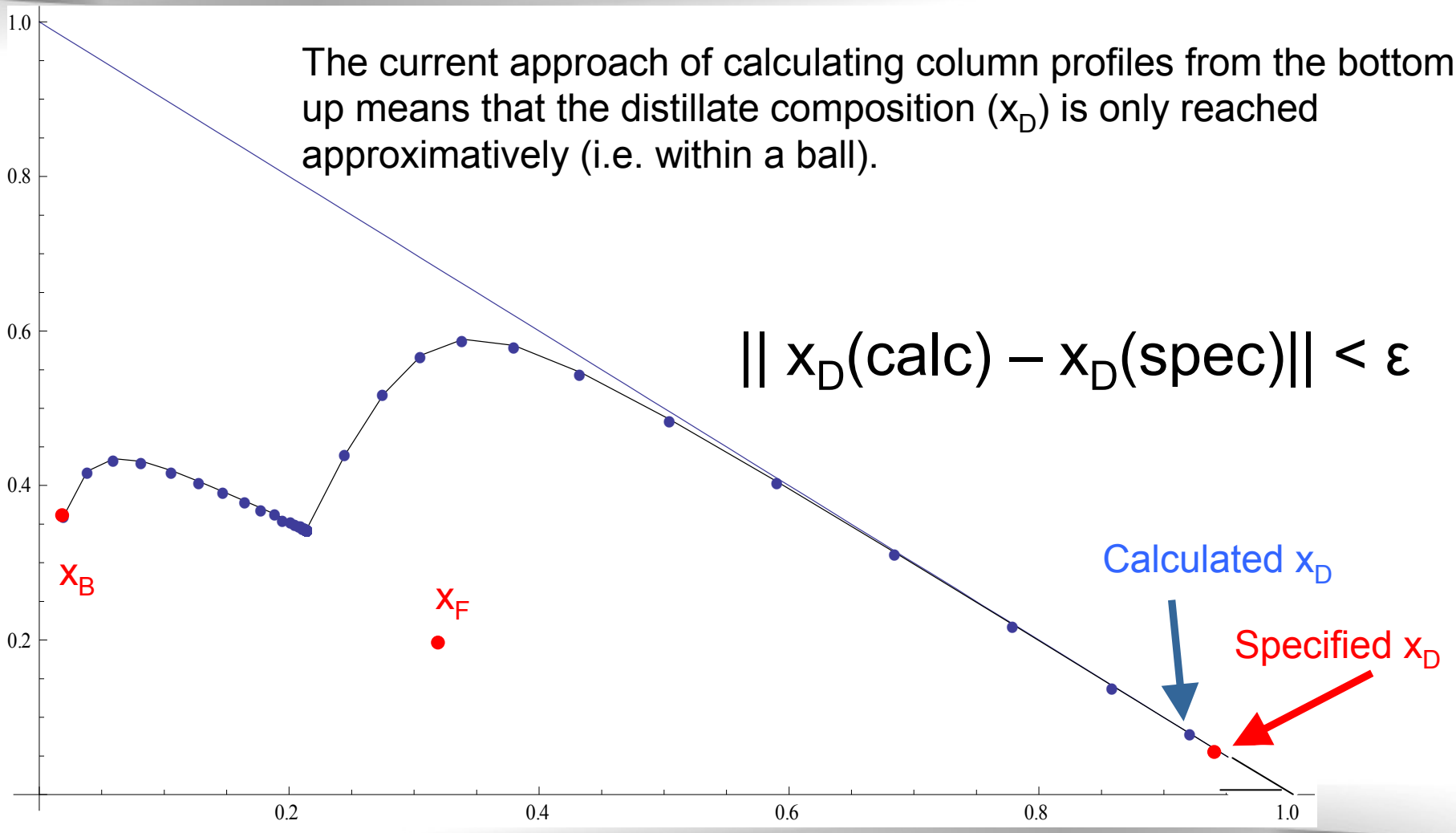
Behaviour for different energy consumptions



Workshop Problem

The current approach of calculating column profiles from the bottom up means that the distillate composition (x_D) is only reached approximatively (i.e. within a ball).

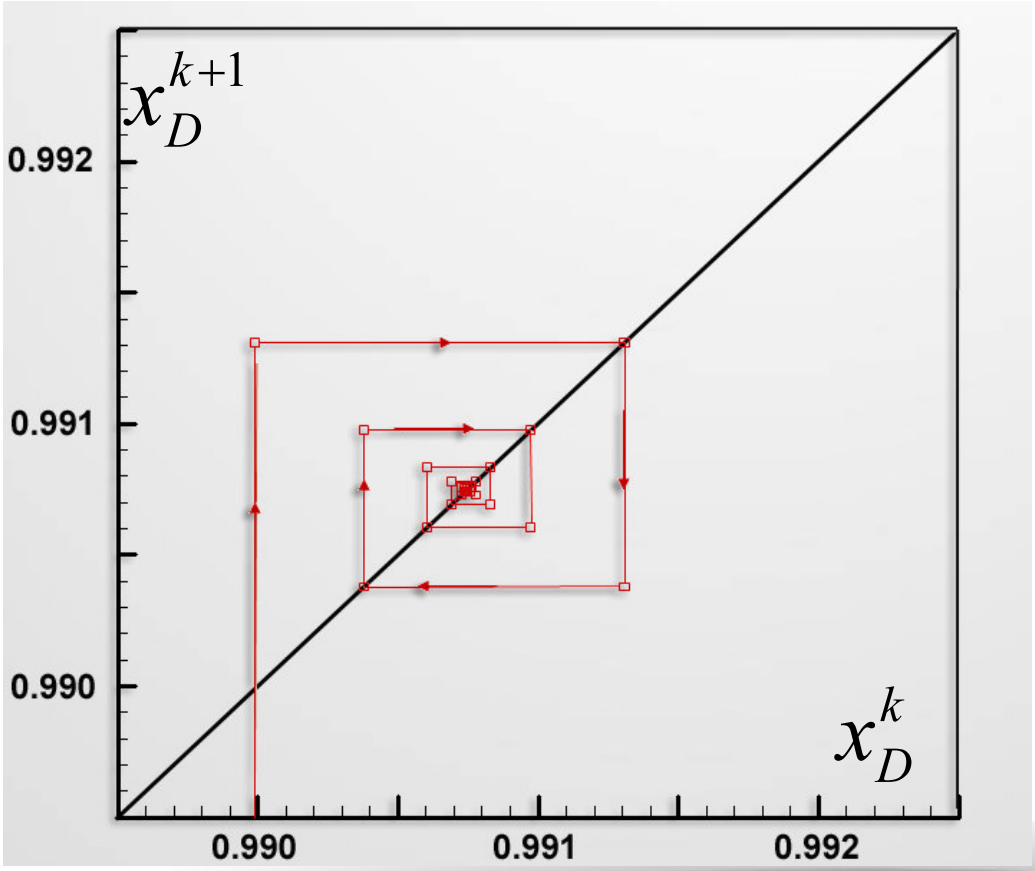
$$|| x_D(calc) - x_D(spec)|| < \varepsilon$$



As a consequence, the optimization algorithm will often propose a solution which satisfies mass balances only approximatively.

Mass balance errors can lead to incorrect decision regarding feasibility (reaching market specified product compositions) and result in increased energy requirements.

These issues can be resolved automatically using direct substitution.



Similar behaviour was observed for many cases (see Lucia et al.).

Refining the optimization results in order to satisfy mass balances can yield a reduction of up to 75% in energy consumption (see Lucia et al.).

Guaranteeing convergence of the successive approximation procedure is therefore important !

Solution Approach

Workgroup goal: prove the mathematical convergence (as opposed to numerical convergence) of the direct substitution procedure towards a unique solution.

Basic observation: If this solution exists, it must be a fixed point of the iterative map.

Questions

- Is the iterative map a contraction?
- Can one calculate the spectrum of its differential?
- Where is the coffee?

Overview of Results

Formulating the problem in a rigorous manner…

… and sparing you the details….

Fixé : x_F, x_B, q, N_s, s.

Soit $r : \Delta^{c-1} \to \mathbb{R}$ déf. par

$$r(y_D) = (s-q+1)\,\frac{y_{D,1} - x_{F,1}}{x_{F,1} - x_{B,1}} - q$$

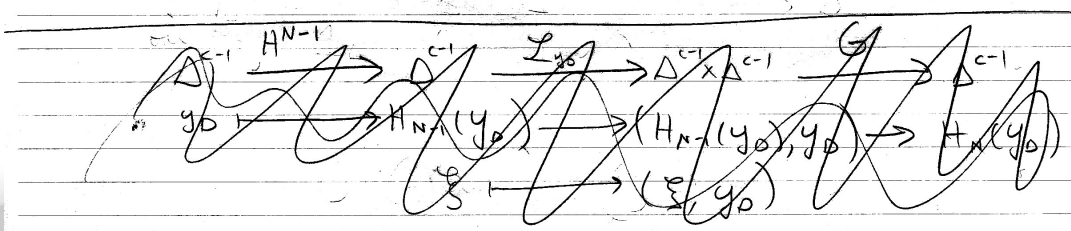
Soit $G : \Delta^{c-1} \times \Delta^{c-1} \to \Delta^{c-1}$ déf. par

$$G(y, y_D) = f\left(\underbrace{\frac{r(y_{D,1})+1}{r(y_{D,1})}\,y - \frac{y_D}{r(y_{D,1})}}_{=: f_{op}(y, y_D)}\right)$$

Soit $x_* \in \Delta^{c-1}$ et $H_N : \Delta^{c-1} \to \Delta^{c-1}$ déf. par

$$H_N(y_D) = \underbrace{G(\cdots G(G(f(*), y_D), y_D), y_D)}_{N}.$$

Rem. $H_N(y_D) = G(H_{N-1}(y_D), y_D)$, $\forall N \geq 2$.



$$J(H_N)(y_0) = J\big(G(H_{N-1}(y_0), y_0)\big)(y_0)$$

$$= J(G)(H_{N-1}(y_0), y_0) \begin{pmatrix} J(H_{N-1})(y_0) \\ I \end{pmatrix}$$

$$= J(f)(f_{op}(y, y_0))\, J(f_{op})(y, y_0) \begin{pmatrix} J(H_{N-1})(y_0) \\ I \end{pmatrix}$$

$$= J(f)(f_{op}(y, y_0)) \left[\frac{r(y_0)+1}{r(y_0)} J(H_{N-1})(y_0) + J_{y_0}(f_{op})(H_{N-1}(y_0), y_0) \right]$$

where $y = H_{N-1}(y_0)$.

1) $\nabla r(y_0) = \left(\underbrace{\frac{S-q+1}{X_{F,1} - X_{B,1}}}_{=: r'}, 0, \dots, 0 \right)$

2) $$\frac{\partial f_{op,i}}{\partial y_{D,j}} = \frac{\partial \left(\left(1 + \frac{1}{r}\right) y_i - \frac{y_{D,i}}{r} \right)}{\partial y_{D,j}}$$

$$= \begin{cases} 0, & j \neq 1 \text{ et } j \neq i \\ \frac{r'}{r^2}(y_{D,i} - y_i), & j = 1 \text{ et } i \neq j \\ -\frac{1}{r}, & i = j \neq 1 \\ \frac{r'}{r^2}(y_{D,i} - y_i) - \frac{1}{r}, & i = j = 1 \end{cases}$$

Thanks to the CRM for the paper…

The Jacobian of the iterative map is given by:

$$J\left(H_{N_r}\right)\left(x_D\right) = J\left(f\right)\left(x_{N_r}\right)\left[\frac{reflux\left(x_D\right)+1}{reflux\left(x_D\right)} J\left(H_{N_r-1}\right)\left(x_D\right) + M\left(y_{N_r-1}, x_D\right)\right]$$

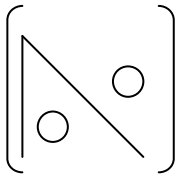
where N_r is the number of distillation trays above the feed

H_j is the vapour composition exiting tray $N_s + j$

f is the equilibrium relation linking liquid and vapor compositions exiting trays

x_j (resp. y_j) is the composition in the liquid (resp. vapour) exiting tray j

reflux is the reflux ratio (flow rate of liquid re-circulated/flow rate of top product)

M is a known matrix with the following structure 

Remark

If the spectral radius of the Jacobian of the iterative map (H_N) is less than 1, then this map is a contraction and therefore the procedure converges to a unique fixed point.

The previous equation gives an indication as to how to calculate this spectrum. It depends only on the eigenvalues of the matrix M and that of the Jacobian of the equilibrium relation (f) – for which studies exist.

Future Work

Properties of the vector field f(x) – x defined by the equilibrium function (f) need to be further investigated (i.e. literature survey).